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CALCULATIONS OF SURFACE BINDING AND
MOBILITY OF ADATOMS

FINAL REPORT

H. B. Huntington

June 23, 1982

U. S. ARMY RESEARCH OFFICE

Contract DAAG29 80 C0130/Grant DAAG29 78 G0065

RENSSELAER POLYTECHNIC INSTITUTE

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19. KEY WORDS (Continue on reverse side if necessary and identify by block number) Adatom, surface, density functional approximation, surface mobility, vicinal crystal.		
20. ABSTRACT (Continue on reverse side if necessary and identify by block number) ✓ Theoretical calculations are developed to explore the behavior of adatoms on the surfaces of a simple metal. The first application was to an adatom (pseudo potential plus valence electron) on a jellium model of a free electron type metal. The density functional approximation was used to evaluate the binding energy as a function of adatom-surface distance. Next a layer of surface ions was introduced and the adatom surface binding energy determined as a function of position over the surface, thereby evaluating the energy for		

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20. ABSTRACT CONTINUED

surface migration. Finally the influence of one layer steps, or ledges, on an otherwise smooth surface, were explored and the size of the binding energy for adatoms at a ledge was evaluated.



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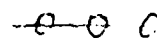

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----- Binding Energy Without Charge Distortions
 ————— Binding Energy with Adatom Polarization

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 Energy Without Charge Distortion
 Energy with Adatom Polarization

The research carried on in this project was concerned with an important aspect of surface physics, namely the behavior of adatoms, whether impurities or self atoms. The research dealt with three aspects of adatom binding and mobility and each aspect is treated in a separate publication. Two of these have been published and the third is in press. They are listed below along with a fourth paper which describes a special treatment for a term difficult to evaluate. All the details of the work are now, or soon will be, available in the open literature. Here only the principal results will be summarized.

List of Publications

- a. "Binding of an Adatom to a Simple Metal Surface", H. B. Huntington, L. A. Turk and W. W. White III, Surface Sci. 48, 186 (1975).
- b. "Local Density Functional for Kinetic Energy", H. B. Huntington, Phys. Rev. B 20, 3165 (1979).
- c. "Adatom Mobility on the Surface of a Simple Metal", A. B. Meador, Te-Hua Lin and H. B. Huntington, Surface Sci. 97, 53 (1980).
- d. "Adatom Binding at the Surface Ledges of a Jellium Metal", M. D. Thompson and H. B. Huntington, Surface Sci., in press for Vol. 116 (3) 522 (1982).

The first stage in this research is summarized in paper (a) and was actually completed prior to ARO support. Here we treated the adatom as an Ashcroft¹ pseudo-potential ion with Herman Skillman² valence electron wave function. For the metal a jellium model was chosen with an electron fall-off at the surface after the procedure of Smith.³ Parameters were chosen to simulate a sodium atom on a sodium surface. The binding energy of adatom on the surface was obtained in first approximation by using the Density Functional Approximation for the combined

atom surface electron distribution as shown by the dashed curve in Fig. 1. The solid curve shows the improvement in the energy obtained by varying the charge distribution of the adatom.

Paper b is the work of the principal investigator aimed to simplify the calculation of the kinetic energy contribution to such problems involving inhomogeneous electron distributions. The research was supported by ARO.

The second phase of this research is reported in paper c, listed above. Here a plane of metal ions has replaced an equivalent slice of the jellium used in (a). The procedure is much the same as before. Two minor changes are the use of a Topp-Hopfield⁴ pseudo-potential which avoids the discontinuity in slope of the Ashcroft form and the change from the Smith³ expression for electron density fall off at the surface to an error function formulation which avoids the discontinuity in the second derivative.

The first step in the calculation is to seek a modulation of the electron distribution parallel to the surface which will minimize the surface energy alone. Next the adatom is allowed to approach the surface and the energies of the adatom are calculated for three symmetric configurations: A directly above an ion of the surface, B directly above a bridge point halfway between surface ions and C above the center point of three or four surface ions. Calculations were performed for four surfaces: (111) and (200) for the fcc lattice and (110) and (200) for the bcc lattice. For these four cases $E_B - E_C$ gives the motion energy for adatom mobility; the diffusion is isotropic over these surfaces.

The most significant result of this investigation became apparent on plotting the various energies, particularly $E_B - E_C$ (see Fig. 2), as a function σ designed to measure the degree of surface close packing. The σ is defined as the ratio of

the square of the interplanar spacing to the area per surface atom. It turns out that all energy quantities appear to depend only on σ and are quite independent, otherwise on surface geometry, i.e. whether the net surface is triangular, square or rectangular. As an example of this, Fig. 2 shows the values of the motion energy for the four surfaces considered plotted versus σ .

The third phase of this work deals with vicinal surfaces, or planes exhibiting an even spacing of atomic ledges. Because of the important implication for catalysis, the binding of the adatoms at the ledges is of interest. The same machinery invoked in paper (b) is also employed here.

The first step in the calculation was to introduce a modulated electron distribution in the neighborhood of the ledges, using many of the devices developed in paper (b). A fall-off parameter, this time associated with the coordinate along the surface perpendicular to the ledges, is determined by minimizing the surface energy.

Next an adatom on the surface is brought in to the ledge, first along the lower terrace and then along the upper terrace. The variation of the energy as a function of position is shown in Fig. 3. The upper curve [O] is obtained by simply superimposing charge distributions. The lower curve [Δ] shows the effect of adatom distortion in lowering the energy. As might be expected, the surface binding energy is increased approaching the ledge from the lower terrace - by about 0.18 eV - whereas approaching the ledge from the upper terrace the adatom binding energy is reduced by about 0.16 eV. There is then an effective "ballustrade" which repulses the adatoms approaching the ledge from the upper terrace while those from the lower terrace are captured to start a new line extending the ledge. As a consequence it can be deduced that, for a vicinal

surface growing, say, by vapor deposition, there will be a tendency to establish a uniform inter-ledge separation.

Participating Scientific Personnel

(These, with one exception, were postdoctoral students so that there are no advanced degrees earned.)

Dr. Willard W. Wright

Dr. Laurence A. Turk

Dr. Albert B. Meador

Mr. Te-Hua Lin

Dr. Michael D. Thompson

Dr. Kshyamasil Patel

Mr. Lin is now completing a doctoral program in experimental surface physics at the University of California (Berkeley) with Professor Somerjai.

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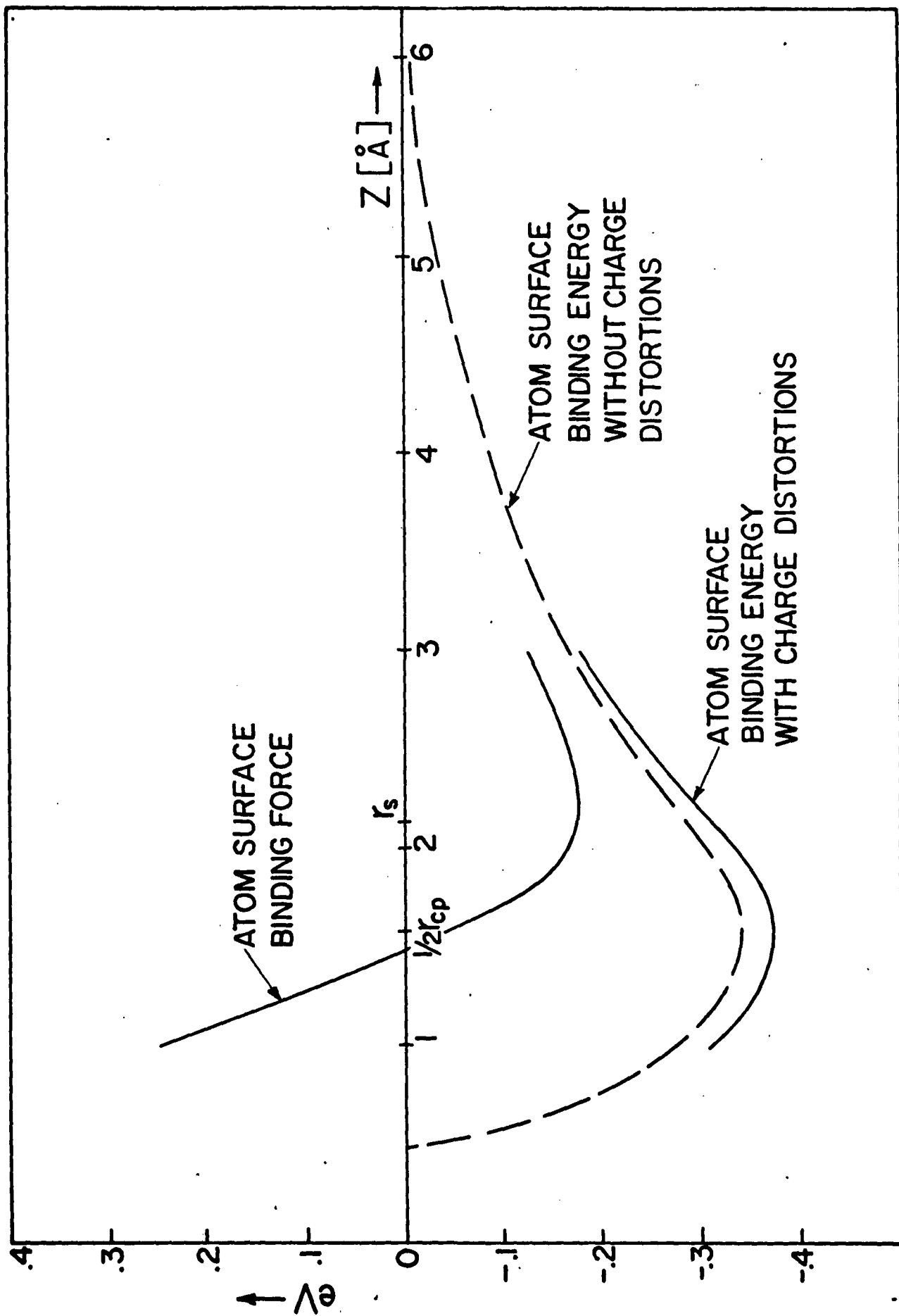


Figure 1.

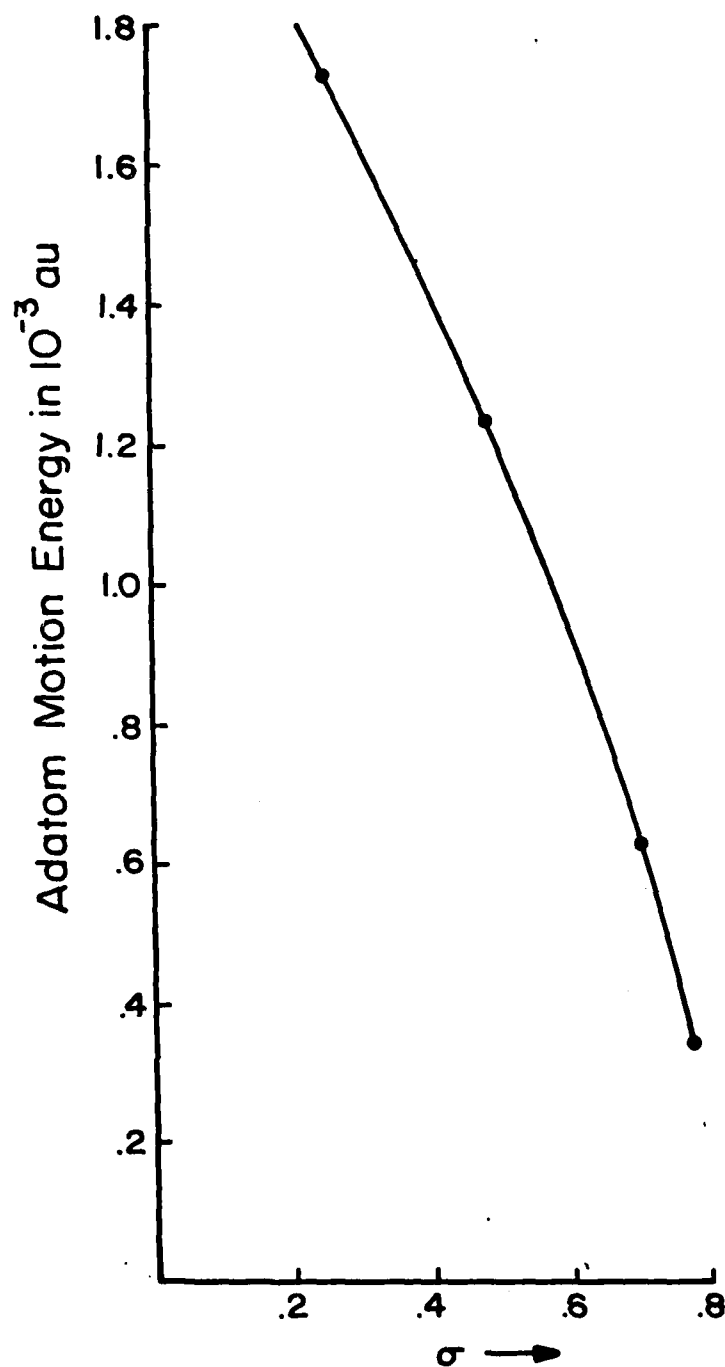


Figure 2. Adatom Motion Energy as a Function of σ , the Close-Packing Surface Parameter.

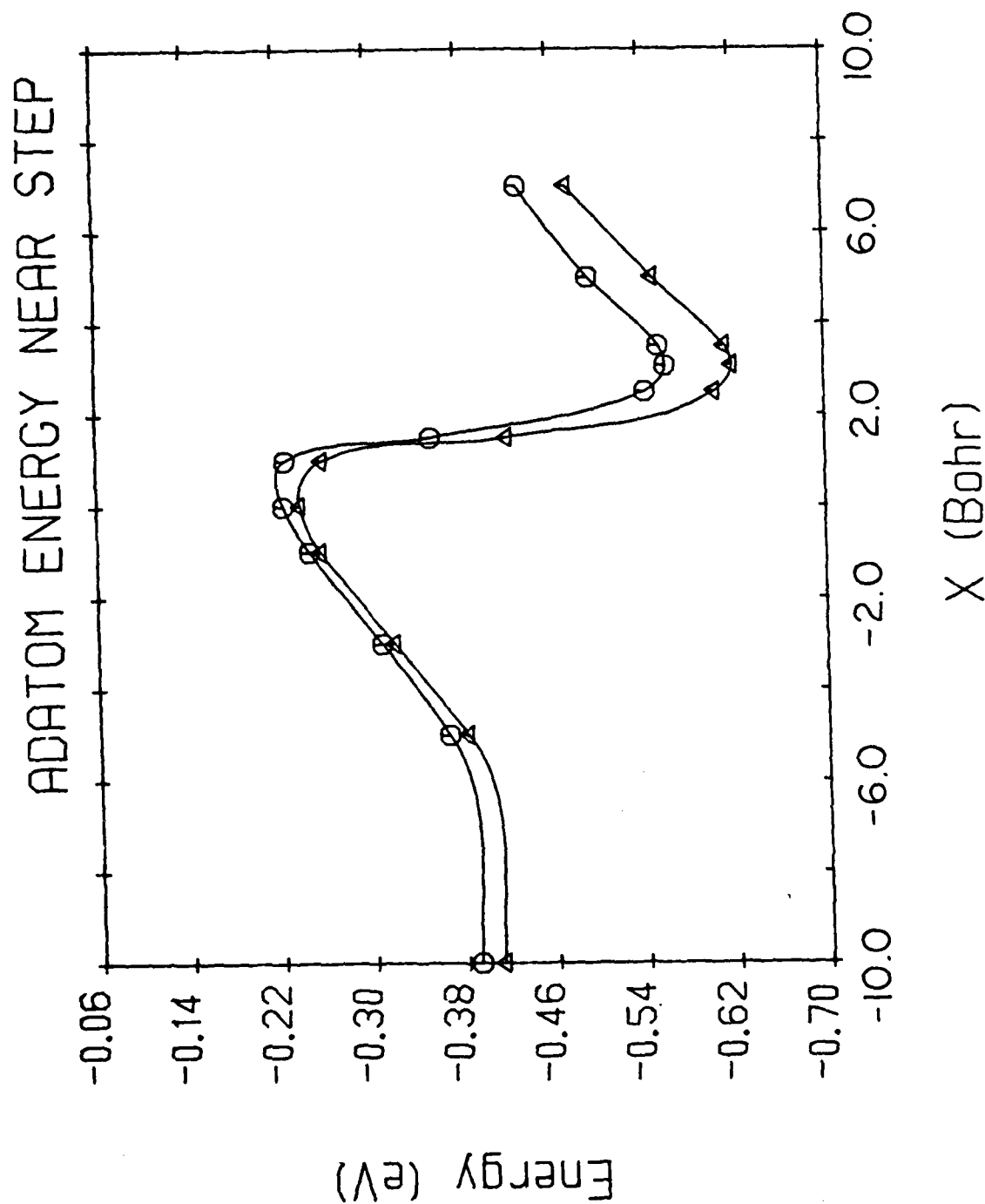


Figure 3. Adatom Energy as a Function of Distance Along the Surface from the Ledge Center.
Energy Without Charge Distortion and Energy with Adatom Polarization.

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